Useful Equations

Time-independent Schrodinger equation of hydrogen

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi_{nlm_\ell}}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi_{nlm_\ell}}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi_{nlm_\ell}}{\partial\phi^2}$$

$$+\frac{2m}{\hbar^2}\left(E_n+\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}\right)\psi_{nlm_\ell}=0$$

Hydrogen in n,ℓ,m_ℓ is described by the wavefunction $\psi_{n\ell m_\ell}=R_{n\ell}(r)Y_{\ell m_\ell}(\theta,\phi)$

$R_{1,0}=\frac{2}{a_0^{3/2}}e^{-r/a_0}$, $R_{2,0}=\frac{1}{2\sqrt{2}a_0^{3/2}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$, $R_{2,1}=\frac{1}{2\sqrt{6}a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$, $Y_{1,\pm1}=\mp\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{\pm i\phi}$,

$Y_{1,0}=\frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$, $Y_{0,0}=\frac{1}{2\sqrt{\pi}}$, $Y_{2,0}=\frac{1}{4}\sqrt{\frac{5}{\pi}}\left(3\cos^2\theta-1\right)$, $Y_{2,\pm1}=\mp\frac{1}{2}\sqrt{\frac{15}{2\pi}}\cos\theta\sin\theta e^{\pm i\phi}$

Bohr radius $a_0=\frac{4\pi\varepsilon_0\hbar^2}{me^2}=5.29\times10^{-11}m$. $E_n=-\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{1}{n^2}=-\frac{13.6eV}{n^2}$, $n=1,2,3\ldots$;

$L=\sqrt{\ell(\ell+1)}\hbar,\ell=0,1,2\ldots n-1$; $L_z=m_\ell\hbar$, $m_\ell=0,\pm1,\pm2,\ldots\pm\ell$. Spin:

$S=\frac{\sqrt{3}}{2}\hbar$, $S_z=m_\ell\hbar$; $m_\ell=+\frac{1}{2}$(up), $-\frac{1}{2}$(down) ; Radial probability: $P_{n\ell}(r)dr=r^2R_{n\ell}^2dr$

Magnetic moment of an electron: $\vec{\mu}_L=-\left(\frac{e}{2m}\right)\vec{L}$ (orbital); $\vec{\mu}_S=-\left(\frac{e}{m}\right)\vec{S}$ (spin). External Magnetic Field, $\vec{B}_{ext}$: $E=-\vec{\mu}\bullet\vec{B}_{ext}$, $\vec{\mu}\equiv$ magnetic moment ; Spherical Coordinate: x = rsinθcosϕ, y = rsinθsinϕ, z = rcosθ; Photon: $E=h\nu$, $\lambda=c/\nu$, $c=3\times10^8m/s$, $h=4.136\times10^{-15}eV\bullet s=6.626\times10^{-34}J\bullet s$ .Fine-Structure Energy $\Delta V_{fs}=2\mu_BB_{\text{int}}$

Zeeman Effect $V_z=g\mu_BB_{ext}m_J$, Lande Factor $g=1+\frac{J(J+1)+S(S+1)-L(L+1)}{2J(J+1)}$

Bohr magneton $\mu_B=\frac{e\hbar}{2m}=5.788\times10^{-5}eV/T$. **Spectroscopic (Term) Symbol** $n^{2S+1}L_J$

Energy order of electron subshell 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s ….

Hund's rule 1) The total spin angular momentum is maximized without violating the Pauli's exclusion principle; 2) Insofar as rule 1 is not violated, L should also be maximized; 3) For an gatom with subshell less than half full, J should be minimized.

More useful constant Mass of electron $9.1\times10^{-31}kg$;

$\hbar=1.054\times10^{-34}J\bullet s=6.5821\times10^{-16}eV\bullet s$. **Addition of Angular Momentum**: $\vec{J}=\vec{L}+\vec{S}$,

$J=L+S,L+S-1,\ldots\left|L-S\right|$, $M_J=\pm J,\pm(J-1),\pm(J-2),\ldots$

Selection rules: 1) **atom with fine structure** $\Delta n\equiv$anything, $\Delta S=0$, $\Delta J=0,\pm1$, $\Delta L=\pm1$ ($J=0\rightarrow J=0$ is not allowed); 2) **Zeeman Effect** $\Delta n\equiv$anything, $\Delta S=0$, $\Delta J=0,\pm1$, $\Delta L=\pm1$ ($J=0\rightarrow J=0$ is not allowed), $\Delta m_J=0,\pm1$ ($m_J=0\rightarrow m_J=0$ is not allowed if $\Delta J=0$)